

10/767,133

=> d his

(FILE 'HOME' ENTERED AT 14:40:05 ON 13 DEC 2004)

FILE 'REGISTRY' ENTERED AT 14:40:52 ON 13 DEC 2004

L1 SCREEN 1996
L2 STRUCTURE UPLOADED
L3 QUE L2 AND L1
L4 0 S L3
L5 9 S L3 FULL

FILE 'CAPLUS' ENTERED AT 14:42:55 ON 13 DEC 2004

L6 6 S L5
L7 6 DUP REM L6 (0 DUPLICATES REMOVED)

FILE 'REGISTRY' ENTERED AT 14:43:38 ON 13 DEC 2004

L8 SCREEN 1996
L9 STRUCTURE UPLOADED
L10 QUE L9 AND L8
L11 0 S L10
L12 5 S L10 FULL

FILE 'CAPLUS' ENTERED AT 14:45:19 ON 13 DEC 2004

L13 6 S L12
L14 6 DUP REM L13 (0 DUPLICATES REMOVED)
L15 6 S L7
L16 6 S L7 NOT L13

FILE 'STNGUIDE' ENTERED AT 14:46:48 ON 13 DEC 2004

FILE 'REGISTRY' ENTERED AT 14:52:47 ON 13 DEC 2004

E HEHA/CN
L17 0 S HEXA(L) AZA(L) CYCLO(L) OCTO(L) DECANE(L) ACETIC(L) ACID
L18 0 S AZA(L) CYCLO(L) OCTO(L) DECANE(L) ACETIC(L) ACID
L19 0 S CYCLO(L) OCTO(L) DECANE(L) ACETIC(L) ACID
L20 1705 S CYCLO(L) DECANE(L) ACETIC(L) ACID

FILE 'CAPLUS' ENTERED AT 14:54:44 ON 13 DEC 2004

L21 6 S L7
L22 996 S L20 OR L7 OR L15
L23 3 S L22 AND (DECONTAMIN? OR DETOX?)
L24 3 DUP REM L23 (0 DUPLICATES REMOVED)

FILE 'REGISTRY' ENTERED AT 14:55:58 ON 13 DEC 2004

E BENZENE/CN
L25 1 S E3

FILE 'CAPLUS' ENTERED AT 14:56:19 ON 13 DEC 2004

L26 7 S L25 AND L22
L27 7 DUP REM L26 (0 DUPLICATES REMOVED)
L28 6 S L6 OR L15
L29 7 S L27
L30 7 S L27 NOT L28

=> log y

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=>Testing the current file.... screen

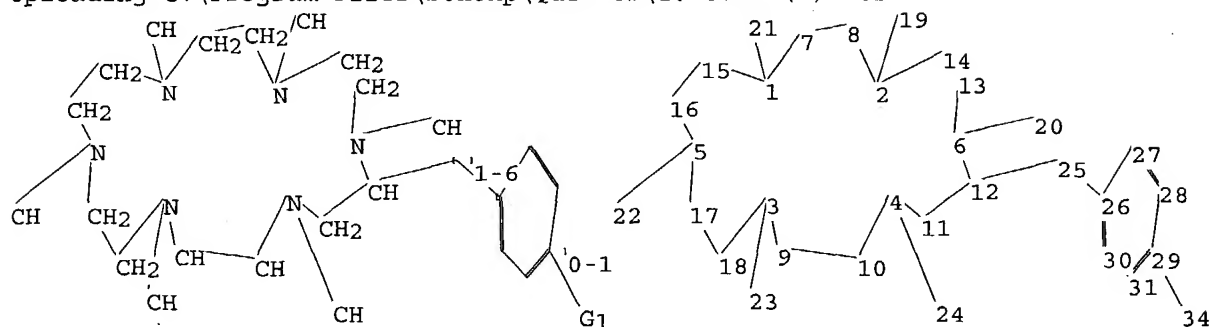
ENTER SCREEN EXPRESSION OR (END):end

=> screen 1996

L1 SCREEN CREATED

=>

Uploading C:\Program Files\Stnexp\Queries\10767133(I).str



chain nodes :

19 20 21 22 23 24 25 34

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 26 27 28 29 30 31

chain bonds :

1-21 2-19 3-23 4-24 5-22 6-20 12-25 25-26 29-34

ring bonds :

1-7 1-15 2-8 2-14 3-9 3-18 4-10 4-11 5-16 5-17 6-12 6-13 7-8 9-10 11-12

13-14 15-16 17-18 26-27 26-30 27-28 28-29 29-31 30-31

exact/norm bonds :

1-7 1-15 1-21 2-8 2-14 2-19 3-9 3-18 3-23 4-10 4-11 4-24 5-16 5-17

5-22 6-12 6-13 6-20 7-8 9-10 11-12 13-14 15-16 17-18 29-34

exact bonds :

12-25 25-26

normalized bonds :

26-27 26-30 27-28 28-29 29-31 30-31

G1:NH2,NO2,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS

20:CLASS 21:CLASS

22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom

31:Atom 34:CLASS

L2 STRUCTURE UPLOADED

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=> que L2 AND L1

L3 QUE L2 AND L1

=> d

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>Testing the current file.... screen

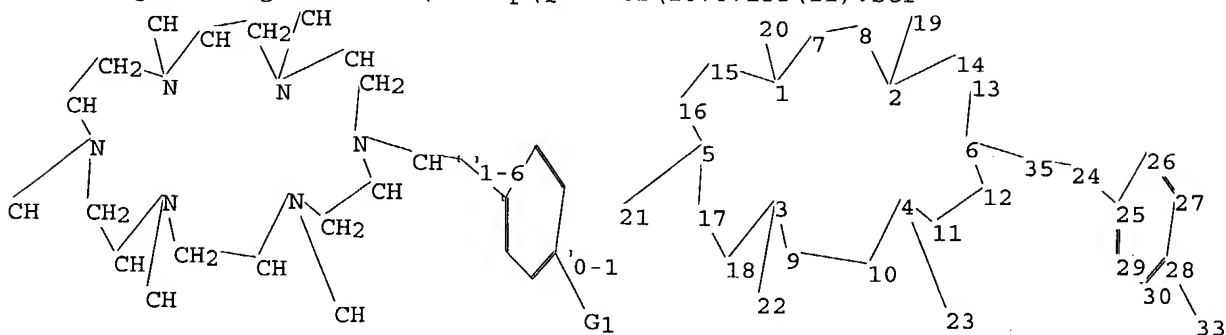
ENTER SCREEN EXPRESSION OR (END):end

=> screen 1996

L8 SCREEN CREATED

=>

Uploading C:\Program Files\Stnexp\Queries\10767133(II).str



chain nodes :

19 20 21 22 23 24 33 35

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 25 26 27 28 29 30

chain bonds :

1-20 2-19 3-22 4-23 5-21 6-35 24-25 24-35 28-33

ring bonds :

1-7 1-15 2-8 2-14 3-9 3-18 4-10 4-11 5-16 5-17 6-12 6-13 7-8 9-10 11-12

13-14 15-16 17-18 25-26 25-29 26-27 27-28 28-30 29-30

exact/norm bonds :

1-7 1-15 1-20 2-8 2-14 2-19 3-9 3-18 3-22 4-10 4-11 4-23 5-16 5-17 5-21 6-12 6-13 6-35 7-8 9-10 11-12 13-14 15-16 17-18 28-33

exact bonds :

24-25 24-35

normalized bonds :

25-26 25-29 26-27 27-28 28-30 29-30

G1:NH2,NO2,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS

20:CLASS 21:CLASS

22:CLASS 23:CLASS 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom

33:CLASS 35:CLASS

L9 STRUCTURE UPLOADED

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=> que L9 AND L8

L10 QUE L9 AND L8